Ecotox Report for Case # P-18-0227

General

[redacted]

Report Status: Complete

Status Date: 10/04/2018

CRSS Date:

SAT Date:

SAT Chair:

Consolidated PMN: N

Consolidated Set:

Ecotox Related Cases: [redacted]

Health Related Cases:

Submitter: [redacted]

CAS Number: 87-73-0

Chemical Name: D-Glucaric acid

Use: Chemical intermediate for [redacted]

Trade Name: KGA50 (product containing the notified substance at [redacted] KGAP

PV-max(kg/yr): [redacted]

Ecotox Assessor: Gallagher, Jeffrey

Fate Summary Statement

Fate Summary Statement: P-18-0227 FATE: [redacted]

[redacted] via
sorption and biodeg
Time for complete ultimate aerobic biodeg = [redacted] wk
Sorption to soils/sediments = low
PBT Potential: P1B1
*CEB
FATE: Migration to ground water = negl
Bioconcentration factor to be put into E-FAST: NA

Physical Chemical Information

Molecular Weight: 210.14

Wt% < 500: **Wt% < 1000:**

Physical State - Neat: Solid

Melting Point: [redacted] **Melting Point (est):**

MP (EPI): [redacted]

Vapor Pressure: **Vapor Pressure (est):** [redacted]

VP (EPI): [redacted]

Water Solubility: [redacted] **Water Solubility (est):** [redacted]

Water Solubility (EPI): [redacted]

Henry's Law:: [redacted]

Log Koc:	[redacted]	**Log Koc (EPI):**	[redacted]
Log Kow:		**Log Kow (EPI):**	
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	2
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	All releases to water

Ecotox Comments

Exposure Based Review (Eco):	N
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1	1		

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):	95-99.9					
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
Fish BCF:	3.16 L/kg wet-wt					
Log Fish BCF:	NaN (Exp.) 0.5 (Est.)					
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:	2	Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	1	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
		Negligible	Slow	Moderate	Rapid	

Removal in WWT/POTW (Overall):	95-99.9					
Condition	**Rating Values**	**Rating Description** 1	2	3	4	**Comment**
Atmospheric Ox B, O3:						
Bio Comments:	The diacid structure drawn represents the solid form of the PMN material. In aqueous solution, the substance exists as the diacid in equilibrium with lactone forms (such as OC(=O)C(O)C1C(O)C(O)C(=O)O1). This equilibrium is transient in nature, incidental to storage of the aqueous solutions, and has no commercial purpose. In addition, the end use of the aqueous solution will generally push the equilibrium back to the diacid form. A fate study summary is available. Fugacity calculations are available. Fish log BAF = -0.05 (1). The fugacity spreadsheet and the EPI output file for the PMN material with manually entered properties are attached.					
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	> 100		ECHA data on 87-69-4
Daphnid	48-h	LC50	93.3		" "
Green Algae	96-h	EC50	51.4		" "
Fish	-	Chronic Value	>10		ECHA data on 87-69-4; ACR of 10
Daphnid	-	Chronic Value	9.33		" "
Green Algae	-	Chronic Value	4.42		ECHA data on 87-69-4

Ecotox Value Comments: Predictions are based on experimental test data on an analogue (CASRN 87-69-4); MW 210; [redacted]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
[redacted]		effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.			

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	51400	4	12850	72hr EC50 Algae
Chronic Aquatic(ppb):	4420	10	442	Algal ChV

Factors	Values	Comments
SARs:		N/A
SAR Class:		N/A
TSCA NCC Category?	Neutral Organics	

Recommended Testing:

Ecotox Factors Comments: Focus

Report/Decision Document:
Environmental Hazard and Risk
(P-18-0227)

Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data on analogues chemicals. Based on these estimated hazard values, EPA concludes that this chemical substance has a moderate environmental hazard.

- Substance falls within the TSCA New Chemicals Categories of neutral organics
- Analogue (CASRN: 87-69-4) was judged to be appropriate for use in assessing this chemical because of structural similarities as well as similarities with respect to physical/chemical characteristics.
- Based on analogue test data, the acute toxicity values estimated for fish, aquatic invertebrates and algae

	are > 100 mg/L, 93.3 mg/L, and 51.4 mg/L, respectively. • Based on analogue test data, the chronic toxicity values estimated for fish, aquatic invertebrates and algae are > 10 mg/L (ACR of 10), 9.33 mg/L (ACR of 10), and 4.42 mg/L, respectively. • These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. • Application of assessment factors of 4 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 12.85 mg/L (12,850 ppb) and 0.442 mg/L (442 ppb), respectively.

Comments/Telephone Log

Artifact	Update/Upload Time